

Appendix A

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<?xml version="1.0" encoding="UTF-8" ?>
- <model name="FieldKorosNoyesModel">
- <notes>
5 <h1>Field-Koros-Noyes Model of BZ Reaction</h1>
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- <thead>
- <tr>
  <th align="left" valign="middle" bgcolor="#eeeeee">Citation</th>
10   </tr>
  </thead>
- <tbody>
- <tr>
- <td>
15   R.J.Field and R.M.Noyes, J.Chem.Phys.60,1877 (1974) ;
    R.J.Field, E.Koros, R.M.Noyes, JACS 94,8649 (1972); R.J.Field, R.M.Noyes, Nature
    237,390 (1972) This implementation is taken manufactured by J.D. Murray,
    "Mathematical Biology" (1989) page 181.
<a href="" />
20   </td>
  </tr>
  </tbody>
  </table>
- <table border="0" cellspacing="0" cellpadding="2">
25 <thead>
- <tr>
  <th align="left" valign="middle" bgcolor="#eeeeee">Description</th>
  </tr>
  </thead>
30 <tbody>
- <tr>
  <td>Field Noyes Version of Belousov- Zhabotinsky Reaction. BrO3 is held
    constant; HOBr is typically ignored, and can be replaced by an empty- set. The
    stoichiometry f is typically taken as 1 / 2 or 1 (denominator 1 or 2 in SBML)
35   .</td>
  </tr>
  </tbody>
  </table>
- <table border="0" cellspacing="0" cellpadding="2">
40 <thead>
- <tr>
  <th align="left" valign="middle" bgcolor="#eeeeee">Rate constant      </th>
  <th align="left" valign="middle" bgcolor="#eeeeee">Reaction</th>
  </tr>
45 </thead>
- <tbody>
- <tr>
  <td>k1 = 1.3</td>
  <td>Br + BrO3 -> HBrO2 + HOBr</td>
50 </tr>

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- <tr>
  <td>k2 = 2000000</td>
  <td>Br + HBrO2 -> HOBr^2</td>
  </tr>
5 <tr>
  <td>k3 = 34</td>
  <td>BrO3 + HBrO2 -> Ce^2 + HBrO2^2</td>
  </tr>
- <tr>
10 <td>k4 = 3000</td>
  <td>HBrO2^2 -> BrO3 + HOBr</td>
  </tr>
- <tr>
  <td>k5 = 0.02</td>
15 <td>Ce -> Br^f</td>
  </tr>
  </tbody>
  </table>
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- <tr>
  <th align="left" valign="middle" bgcolor="#eeeeee">Variable</th>
  <th align="left" valign="middle" bgcolor="#eeeeee">IC</th>
  <th align="left" valign="middle" bgcolor="#eeeeee">ODE</th>
25  </tr>
  </thead>
- <tbody>
- <tr>
  <td>Br</td>
30 <td>0.003</td>
  <td>Br'[t] == -(k1*Br[t]*BrO3[t]) + f*k5*Ce[t] - k2*Br[t]*HBrO2[t]</td>
  </tr>
- <tr>
  <td>Ce</td>
35 <td>0.05</td>
  <td>Ce'[t] == -(k5*Ce[t]) + 2*k3*BrO3[t]*HBrO2[t]</td>
  </tr>
- <tr>
  <td>HBrO2</td>
40 <td>0.001</td>
  <td>HBrO2'[t] == k1*Br[t]*BrO3[t] - k2*Br[t]*HBrO2[t] +
    k3*BrO3[t]*HBrO2[t] - k4*HBrO2[t]^2</td>
  </tr>
- <tr>
  <td>HOBr</td>
45 <td>0</td>
  <td>HOBr'[t] == k1*Br[t]*BrO3[t] + 2*k2*Br[t]*HBrO2[t]
    + k4*HBrO2[t]^2</td>
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50 </tbody>
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- <listOfProducts>
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- <reaction name="Reaction2" reversible="false">
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45 </kineticLaw>
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- <listOfProducts>

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